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Testing of RANS turbulence models for stratified flows based on DNS data

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1. Motivation and objectives

Stably stratified flows such as those in the atmosphere or in large water bodies such as the ocean, lakes, estuaries and reservoirs are prevalent in the natural environment. The presence of the buoyancy force due to the stratification may have a substantial effect on the flow development and mixing processes, and hence influence the distribution of scalar substances such as pollutants, suspended sediments, in the environment.

Today, there exist numerous turbulence models for calculating turbulent mixing in the environment. These models range from the simple eddy viscosity models to the more detailed large eddy simulations (LES) and direct numerical simulations (DNS) (Axell & Liungman 2001). However, both DNS and LES can be too computationally expensive (and often too idealized) for most geophysical and engineering applications. This limitation has restricted modelers to RANS approaches commonly based on turbulent kinetic energy (TKE) closure schemes. The most widely used RANS models today are two equation models which solve two transport equations for the properties of the turbulence from which the eddy viscosity can be computed. The best known of these models is the $k-\epsilon$ model which requires the solutions of the turbulent kinetic energy equation (a component of essentially all current multi-equation models) and dissipation of turbulent kinetic energy equation (Ferziger *et al.* 2003).

In most geophysical flows, turbulence occurs at the smallest scales and one of the two most important additional physical phenomena to account for is stratification (the other being rotation). In this paper, the main objective is to investigate proposed changes to RANS turbulence models which include the effects of stratification more explicitly. These proposed changes were developed using a DNS database on stratified and sheared homogenous turbulence developed by Shih *et al.* (2000) and are described more fully in Ferziger *et al.* (2003). The data generated by Shih *et al.* (2000) (hereinafter referred to as SKFR) are used to study the parameters in the $k-\epsilon$ model as a function of the turbulent Froude number, Fr_k . A modified version of the standard $k-\epsilon$ model based on the local turbulent Froude number is proposed. The proposed model is applied to a stratified open channel flow, a test case that differs significantly from the flows from which the modified parameters were derived. The turbulence modeling and results are discussed in the next two sections followed by suggestions for future work.

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2. Turbulence modeling based on DNS data

2.1. The Data

The DNS data of SKFR are used to develop parameterizations of modeling coefficients typically found in RANS models (e.g. C_μ) as functions of quantities that define the local state of the turbulence (Fr_k etc.).

SKFR performed DNS of stratified homogeneous turbulent shear flows. The data have been extensively discussed by SKFR and hence the discussion will not be repeated here. However, it is important to realize that the data provide all of the properties of the turbulence up to second order statistics. The subset of the data used in this study consists of the highest initial Taylor microscale Reynolds number runs ($Re_{\lambda_0} = 89$). The value of $Re_{\lambda_0} = 89$ is relatively high for direct numerical simulations but not high enough to produce results that are independent of Reynolds number effects. It is nevertheless, high enough that the effects of the other parameters should be accurately represented. All the data used for this study were taken from the latter parts of the SKFR runs in order to ensure that the turbulence was fully developed. The physical time was non-dimensionalized as St where S is the shear rate defined as:

$$S = \frac{\partial U}{\partial z} \quad (2.1)$$

As discussed by Ferziger *et al.* (2003), the turbulence does not become fully developed until sometime later than $St > 2$. Most of the runs were continued until $St = 12-14$. In our present study, only the data for times between $St = 8$ and the end of the run were used. To render the plots less confusing, the data is averaged over this time period. In total, 37 runs were used to derive the results given below. Each run is characterized by the initial Reynolds number (which is the same for all the runs) and the gradient Richardson Ri_g (defined in equation 2.2) which has a fixed value for each run.

$$Ri_g = \frac{N^2}{S^2} \quad (2.2)$$

where N is the buoyancy frequency defined as:

$$N = \left(\frac{-g}{\rho} \frac{\partial \rho}{\partial z} \right)^{1/2} \quad (2.3)$$

2.2. $k-\epsilon$ model

$k-\epsilon$ is a commonly used two equation model, of which many variations have been suggested. Here, we base our proposed modifications on the standard version of the $k-\epsilon$ model. In the presence of stratification, the turbulent kinetic energy equation can be written as:

$$\frac{Dk}{Dt} = P - \epsilon - B + D_k \quad (2.4)$$

where P is the rate of production of TKE, which is given, for simple shear flows like the SKFR flows, by:

$$P = -\overline{w'w'}S \quad (2.5)$$

B is the buoyancy flux given by:

$$B = -\frac{g}{\rho_0} \overline{\rho'w'}. \quad (2.6)$$

C_μ	$C_{\epsilon 1}$	$C_{\epsilon 2}$	σ_k	σ_ϵ
0.09	1.44	1.92	1.0	1.3

TABLE 1. Values of constants in the k - ϵ model (Rodi, 1980)

D_k is the transport term (equal to zero for the SKFR flows) modeled using the gradient-diffusion hypothesis as:

$$D_k = \frac{\partial}{\partial z} \left(\frac{\nu_t}{\sigma_k} \frac{\partial k}{\partial z} \right) \quad (2.7)$$

and ϵ , the rate of dissipation of the turbulent kinetic energy, is modeled in an analogous way to equation (2.4):

$$\frac{D\epsilon}{Dt} = C_{\epsilon 1} \frac{P\epsilon}{k} - C_{\epsilon 2} \frac{\epsilon^2}{k} - C_{\epsilon 3} \frac{B\epsilon}{k} + D_\epsilon \quad (2.8)$$

where D_ϵ is the transport term (equal to zero for the SKFR flows) modeled again using the gradient-diffusion hypothesis as:

$$D_\epsilon = \frac{\partial}{\partial z} \left(\frac{\nu_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial z} \right) \quad (2.9)$$

The eddy viscosity is then given by:

$$\nu_t = C_\mu \frac{k^2}{\epsilon} \quad (2.10)$$

and the eddy diffusivity is:

$$\kappa_t = \frac{\nu_t}{Pr_t} \quad (2.11)$$

where Pr_t is the turbulent Prandtl number. The constants that are commonly used are given in Table 1.

The value for the buoyancy parameter $C_{\epsilon 3}$ is a matter of much discussion. Various values have been suggested, e.g. Rodi (1987) suggests a value of $0 < C_{\epsilon 3} < 0.29$, Baum & Caponi (1992) suggest $C_{\epsilon 3} = 1.14$ and Burchard & Baumert (1995) have argued that $C_{\epsilon 3}$ should have negative values. It turns out from our studies that this is a very sensitive parameter for stratified flows.

2.3. Proposed parametrizations

Several parameters have been suggested to characterize the effects of the stratification, the most obvious of which is the gradient Richardson number defined in equation (2.2). However, Ferziger *et al.* (2003) argue that this is not the best choice as it represents the forcing rather than the properties of the turbulence. As pointed out by SKFR, the turbulent Froude number gives better correlations. It can be defined based on the quantities computed from the k - ϵ model as:

$$Fr_k = \frac{\epsilon}{Nk} \quad (2.12)$$

Further, it is also noted that there is a gradient Richardson number at which turbulence

energy neither grows nor decays called the stationary Richardson number Ri_{gs} . Holt *et al.* (1992) showed that Ri_{gs} is a function of the Reynolds number at least at smaller values of Re . If, in equations (2.4) and (2.8), we set $Dk/Dt = D\epsilon/Dt = 0$, and eliminate ϵ , then for homogeneous flows, the following relation is obtained:

$$Ri_{fs} = \frac{B}{P} = \frac{C_{\epsilon 2} - C_{\epsilon 1}}{C_{\epsilon 2} - C_{\epsilon 3}} \quad (2.13)$$

where Ri_{fs} is the flux Richardson number. Applying the gradient diffusion modeling concept to both B and P in equation (2.13) yields:

$$Ri_{fs} = \frac{Ri_{gs}}{Pr_t} \quad (2.14)$$

where it is found that $Pr_t \approx 1$ in the stationary flow cases. Hence we assume that Ri_{fs} and Ri_{gs} are equivalent in the discussion that follows.

We choose to insist that $C_{\epsilon 3}$ be zero at the stationary state in order to satisfy the constraint that the model predicts the existence of a stationary state under the conditions determined by SKFR. Rearranging equation (2.13) and using the generally accepted value of 0.25 for the stationary Richardson number at high turbulence Reynolds number, we get:

$$C_{\epsilon 2} = \frac{C_{\epsilon 1}}{1 - Ri_{fs}} \quad (2.15)$$

The functional dependence of the stationary Richardson number Ri_{gs} on the turbulence Reynolds number Re_k defined in equation (2.16) was given by SKFR as shown in equation (2.17).

$$Re_k = \frac{k^2}{\epsilon \nu} \quad (2.16)$$

$$Ri_{fs} \approx Ri_{gs} = \frac{0.25}{1 + 103/Re_k} \quad (2.17)$$

Any of the parameters in the model ϵ equation can be allowed to vary as a function of the turbulent Froude number but only one parameter (or combination of parameters) can be derived from the model dissipation equation and the DNS data, enforcing a limitation on the choices that can be made. In this study, the parameters that are chosen to depend on the stratification are $C_{\epsilon 3}$ and C_μ , while $C_{\epsilon 1}$ and $C_{\epsilon 2}$ are independent of the stratification. We do however include the effect of the Reynolds number on $C_{\epsilon 2}$ as discussed earlier through equations (2.15) and (2.17).

The buoyancy parameter $C_{\epsilon 3}$ can be calculated from DNS data using the model ϵ equation as a function of Fr_k . To accomplish this, we compute $(1/\epsilon)d\epsilon/dt$ from the SKFR data by fitting a least square straight line to $\log \epsilon$ as a function of time over the time range used in all of the data fitting. We then solve equation (2.8) for $C_{\epsilon 3}$ using equation (2.15) for $C_{\epsilon 2}$ (as discussed by Ferziger *et al.*, 2003). The resulting values are plotted in Figure 1. Unfortunately, there is no clear trend in the data to suggest any definitive fit. However, the data indicates that $C_{\epsilon 3}$ is of order unity in the strongly stratified region and possibly shows a slight increase with increasing Fr_k . The fit we used for this study is also shown in Figure 1 and is given by equation (2.18). This correlation is based on the observation that the mixing efficiency peaks at about Fr_k of 0.4 - 0.5 for the SKFR data and $C_{\epsilon 3}$ should be zero there. It should be noted that the data does not extend into the very strongly stratified regime (i.e. very low Fr_k values). It is a regime that has a

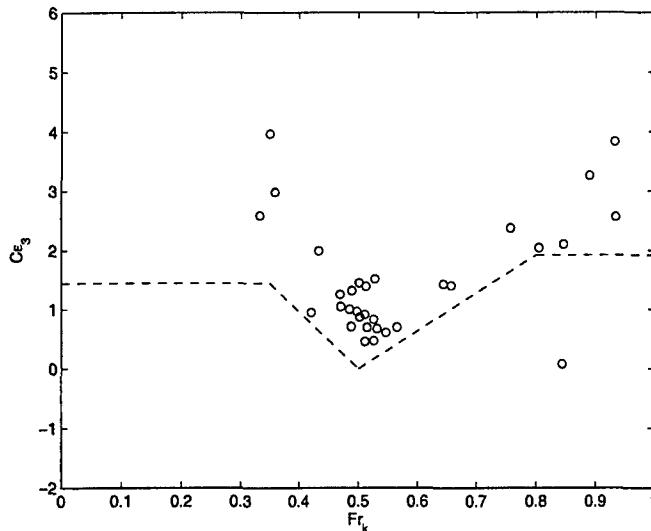


FIGURE 1. Buoyancy parameter $C_{\epsilon 3}$ as a function of the turbulent Froude number. o: values calculated from the SKFR data, ---: fit given by (2.18).

mixture of internal waves and turbulence and care has to be exercised in applying any turbulence model in this regime.

$$C_{\epsilon 3} = \begin{cases} 1.44 & \text{for } Fr_k < 0.35 \\ 1.44 - 9.6(Fr_k - 0.35) & \text{for } 0.35 < Fr_k < 0.50 \\ 6.4(Fr_k - 0.5) & \text{for } 0.5 < Fr_k < 0.80 \\ 1.92 & \text{for } Fr_k > 0.80 \end{cases} \quad (2.18)$$

We note that Figure 1 indicates that a better fit to the data could be given but we felt it important to repeat the condition that $C_{\epsilon 3}$ be zero at $Fr_k = 0.5$.

The eddy viscosity parameter C_μ obtained from the data is plotted as function of Fr_k in Figure 2. The value of C_μ obtained from the SKFR data at large Fr_k (weak stratification) is lower than the typical value of 0.09. However, we fit the data such that C_μ reaches the asymptotic value of 0.09 at high Fr_k values. Thus:

$$C_\mu = \begin{cases} 0.125Fr_k^2 + 0.014Fr_k & \text{for } Fr_k < 0.35 \\ 0.006(Fr_k - 0.35)/(0.02 + 0.1(Fr_k - 0.35)) + 0.02 & \text{for } 0.35 < Fr_k < 0.60 \\ 0.08\tanh(Fr_k) + 0.01 & \text{for } Fr_k > 0.60 \end{cases} \quad (2.19)$$

The scalar transport can be modeled using the turbulent Prandtl number defined in equation (2.11). We plotted the turbulent Prandtl number as a function of the turbulent Froude number as shown in Figure 3. The curve fit shown in the figure is:

$$Pr_t = \begin{cases} 1.4 & \text{for } Fr_k < 0.35 \\ 1.4 - 0.55(1 - \exp(-7(Fr_k - 0.35))) & \text{for } Fr_k > 0.35 \end{cases} \quad (2.20)$$

where we have chosen to keep the Prandtl number constant in the highly stratified regions.

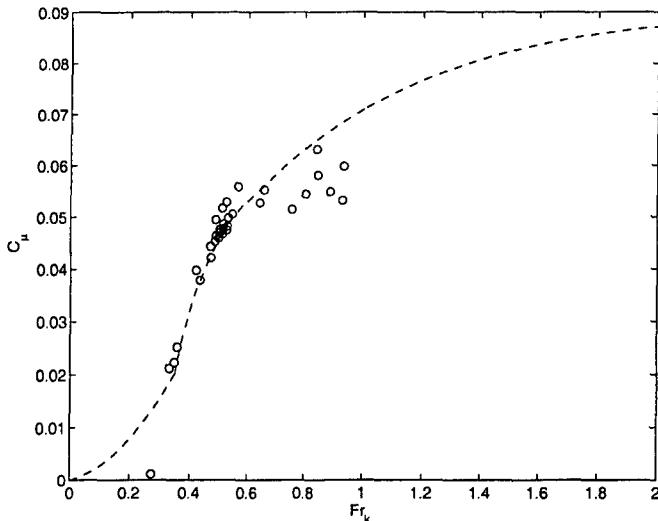


FIGURE 2. The eddy viscosity coefficient C_μ as a function of the turbulent Froude number. o: values derived from the SKFR data, - - - : correlation (2.19)

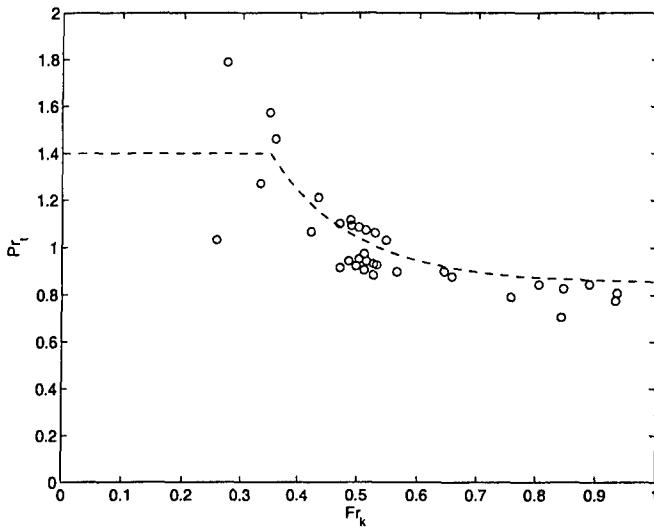


FIGURE 3. The turbulent Prandtl number as a function of the turbulent Froude number. o: values derived from the SKFR data, - - - : correlation (2.20)

3. Results and discussion

In order to test the proposed parameterization and compare it with other models, it is essential that we apply it to a flow that is significantly different from the homogenous flows from which the parameters were derived. We chose the stratified open channel flow as our test case. This is a flow for which direct numerical simulations and large eddy simulations have been performed by Garg *et al.* (2000) and Shih (2003).

The tests of the model were performed using a 1-D water column model called GOTM

(General Ocean Turbulence Model) developed by Burchard *et al.* (1999). The various turbulence closure schemes in GOTM are based on a modular format that enables easy incorporation in 3-D ocean circulation models and also allows for refinements or extensions to the turbulence models. The source code is available to the public on the Internet website www.gotm.net. We incorporated our proposed model into the GOTM code. Since none of the built in stability functions in GOTM modify their parameters based on depth, we had to adapt the code to modify the parameters in $k-\epsilon$ model discussed above to be depth dependent based on the local turbulent Froude number.

The test case we use is somewhat artificial. It is a pressure-gradient driven open channel flow in which the density is held fixed at both the lower solid boundary and the upper free surface and in some ways similar to the experiments done by Komori *et al.* (1983). The Reynolds number Re_t and the Richardson number Ri_t based on the shear velocity for all the test runs were 682 and 31 respectively. Previous studies by Garg *et al.* (2000) have shown that LES produces results that are in good agreement with DNS results for open channel flows. Hence we use an LES run with identical conditions to those in our test case to assess the predictions of our proposed model and that of the standard $k-\epsilon$ model with constant stability functions.

The flow was first allowed to develop to a converged solution (without stratification effects) using the standard $k-\epsilon$ model after which the stratification was imposed. The velocity and density profiles at the initial state (i.e. after spin up) are shown in Figure 4. Also shown in Figure 4, are the turbulent kinetic energy and dissipation profiles together with the turbulent Froude number and the turbulent Reynolds number profiles. Superimposed on these figures are the instantaneous LES profiles.

A total of four runs were done using different combinations of the modifications (outlined above) to the $k-\epsilon$ model so as to determine the most suitable combination of parameters that can match as closely as possible the LES results. The test runs discussed in this paper are outlined in Table 2. Run 1 is based the standard $k-\epsilon$ model with $C_{\epsilon 3} = 1.44$, while run 2 uses the proposed parametrizations. In run 3, we vary only the eddy viscosity parameter C_μ and turbulent Prandtl number Pr_t and keep both $C_{\epsilon 2}$ and $C_{\epsilon 3}$ constant as in run 1. Run 4 is an arbitrary case that was chosen to investigate the effects of just varying the turbulent Prandtl number using the correlation given by equation (3.1).

The velocity, density, turbulent kinetic energy, dissipation of the turbulent kinetic energy, turbulent Froude number and turbulent Reynolds number profiles at non-dimensional times $tu_*/h = 4.1$ and $tu_*/h = 14.6$ for the standard $k-\epsilon$ model (run 1) and the full modified version (run 2) together with the LES profiles are shown in Figures 5 and 6 respectively.

The full modified version of the proposed model (denoted by run 2) underperforms the $k-\epsilon$ model in terms of predicting the velocity profile in the channel especially at later times, as seen in Figure 6, even though it appears to capture the free surface velocity better. However, it does significantly better in predicting the evolution of the density profile, especially during the transient stages of the flow.

In run 3, both $C_{\epsilon 2}$ and $C_{\epsilon 3}$ are held at constant values equal to the ones used for the $k-\epsilon$ test run 1. It can be seen from the density profile in Figure 7 that the mixing is now predicted better for the highly stratified regions (i.e. low Froude numbers) in this run. However, this case underperforms the standard $k-\epsilon$ case for most of the lower half of the channel depth. The discrepancy between the LES and the RANS results given by runs 1 and 3 for the lower half of the channel depth indicates that in general the $k-\epsilon$ model allows too much mixing to occur from the bottom boundary. There is a strong

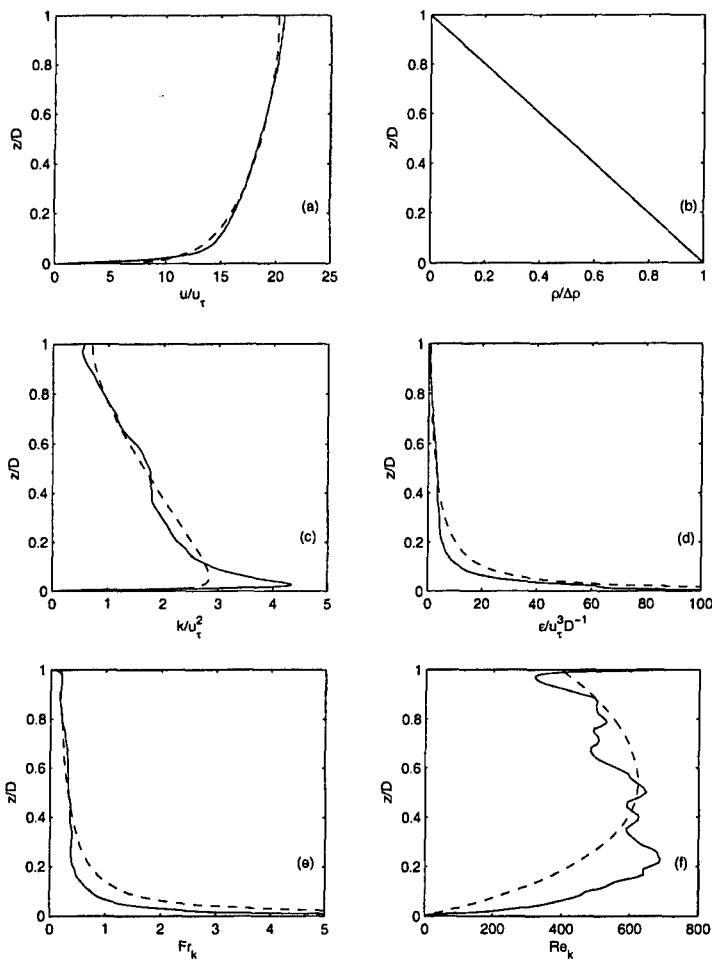


FIGURE 4. Initial profiles (a) velocity; (b) density; (c) tke; (d) dissipation; (e) turbulent Froude number Fr_k ; (f) turbulent Reynolds number Re_k . — : LES results, - - - : $k-\epsilon$ results.

Run	C_μ	$C_{\epsilon 2}$	$C_{\epsilon 3}$	Pr_t	Remarks
1	0.09	1.92	1.44	0.85	Standard $k-\epsilon$ model
2	eq.(2.19)	eq. (2.15)	eq. (2.18)	eq. (2.20)	Full modified version
3	eq.(2.19)	1.92	1.44	eq. (2.20)	Varying C_μ and Pr_t only
4	0.09	1.92	1.44	eq. (3.1)	Varying Pr_t only

TABLE 2. Test runs used for evaluating the predictions by the modified $k-\epsilon$ model

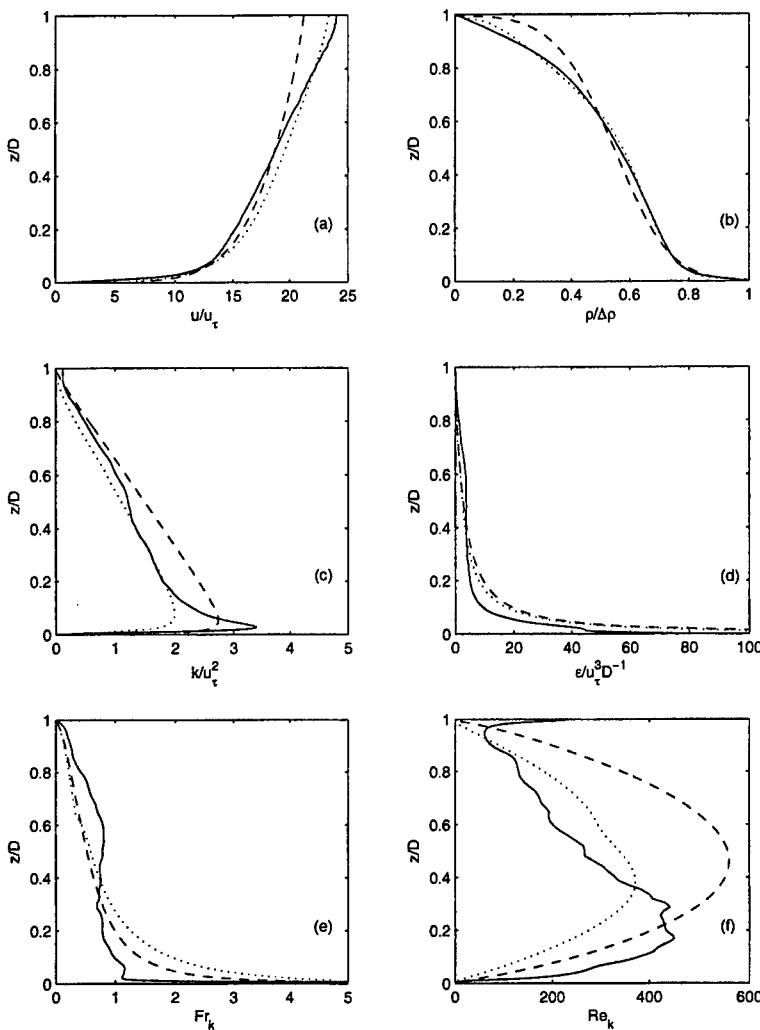


FIGURE 5. Profiles at $tu_*/h = 4.1$: (a) velocity; (b) density; (c) tke; (d) dissipation; (e) Fr_k ; (f) Re_k . — : LES results; - - - : run 1; ··· : run 2.

possibility that the prescribed asymptotic value of 0.85 that the SKFR data suggests for the turbulent Prandtl number is low even though there are good engineering data that suggest this value is reasonable. However, other observations such as those due to Högstrom (1996) suggest a value of $Pr_t = 1$. In run 4, we use a different correlation for Pr_t such that it asymptotes to 1.0 at high Fr_k (see equation 3.1). The results as shown in Figure 7 indicate closer agreement with the LES results compared to runs 1 and 3 respectively. .

$$Pr_t = 0.4 \exp(-2.5 Fr_k) + 1.0 \quad \text{for all } Fr_k \quad (3.1)$$

4. Conclusions and future work

Modifications of the k - ϵ model to account for stratification based on the SKFR data have been suggested and tested in this study. The test runs done on the stratified open

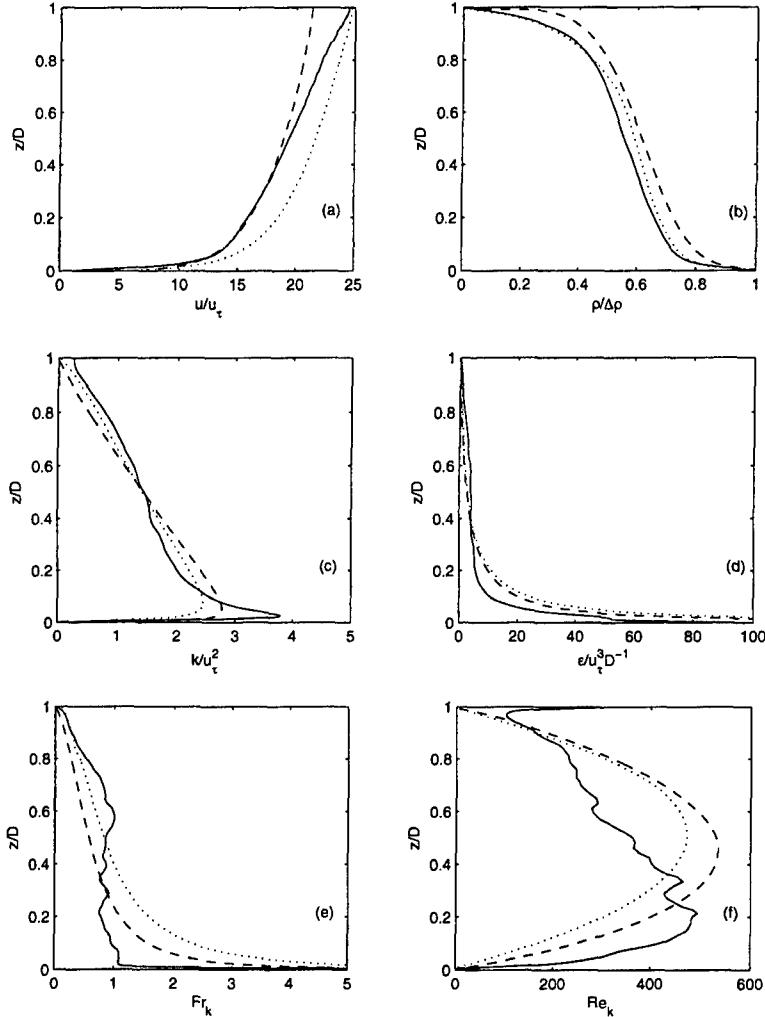


FIGURE 6. Profiles at $tu_*/h = 14.6$: (a) velocity; (b) density; (c) tke; (d) dissipation; (e) Fr_k ; (f) Re_k . — : LES results; - - - : run 1; ... : run 2.

channel flow highlight the importance of correctly modeling the turbulent Prandtl number Pr_t as well as the buoyancy parameter $C_{\epsilon 3}$. The results suggest that the turbulent Prandtl number should be close to unity for the neutrally stable flows. Further, it appears that the buoyancy parameter $C_{\epsilon 3}$ has to be prescribed as a value of the order of $C_{\epsilon 1}$ in order to correctly model the effects of the buoyancy force in the dissipation equation. The lack of a clear trend in $C_{\epsilon 3}$ as a function of Fr_k from the DNS data suggests that the strategy of setting $C_{\epsilon 3}$ equal to a constant is probably the most reasonable approach. The results of this paper are useful only in the regimes of weak to moderate stratification. Clearly further test cases should be performed where the effects of the stratification are more pronounced and where Fr_k is small over larger fraction of the flow depth. This will allow us to evaluate the effects of varying C_μ as function of Fr_k more precisely. Further work is also required to capture the boundary layer dynamics properly so that momentum balance can be achieved properly. We are also unable to comment on the transport models

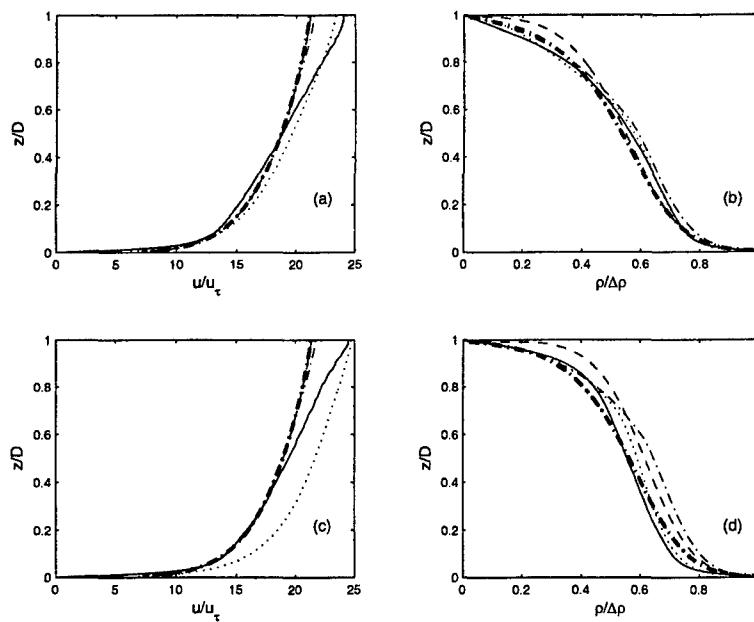


FIGURE 7. Velocity profiles (left) and density profiles (right). — : LES results; - - - : run 1; ... : run 2; - · - : run 3; - · - in bold : run 4 at $tu_*/h = 4.1$ (top) and $tu_*/h = 14.6$ (bottom).

(which may also depend on stratification) as the SKFR database is for homogeneous flows. It is important to obtain data for strongly stratified and inhomogeneous flows and apply them to the development of better models for stably stratified flows.

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